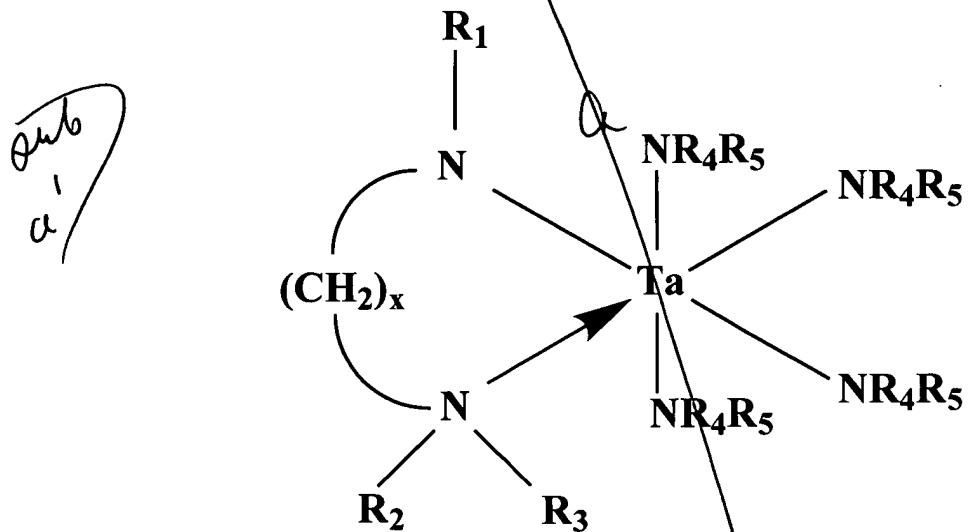


THE CLAIMSWHAT IS CLAIMED IS:

5 1. A source reagent composition comprising at least one tantalum and/or titanium species selected from the group consisting of:

(i) tethered amine tantalum complexes of the formula:



wherein:

x is 2 or 3;

each of R<sub>1</sub>-R<sub>5</sub> is independently selected from the group consisting of H, C<sub>1</sub>-C<sub>4</sub> alkyl, aryl, C<sub>1</sub>-C<sub>6</sub> perfluoroalkyl and trimethylsilyl;

(ii)  $\beta$ -diimines of the formula:

wherein:

5 G is a  $\beta$ -diimino ligand;each Q is selected from the group consisting of H, C<sub>1</sub>-C<sub>6</sub> alkyl, aryl and C<sub>1</sub>-C<sub>6</sub> perfluoroalkyl; and

x is an integer from 1 to 4 inclusive;

## 10 (iii) tantalum diamide complexes of the formula



wherein:

x is 1 or 2;

15 y is 1 or 2;

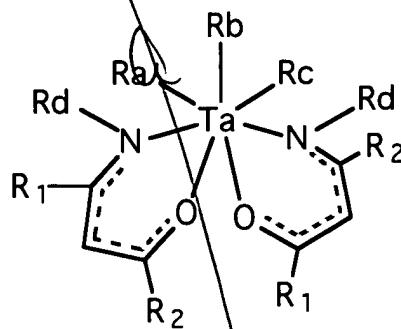
each of R<sub>1</sub>-R<sub>4</sub> is independently selected from the group consisting of H, C<sub>1</sub>-C<sub>4</sub> alkyl, aryl, perfluoroalkyl, and trimethylsilyl;

## (iv) tantalum amide compounds of the formula



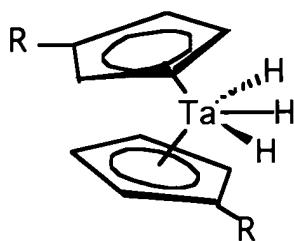
wherein each R and R' is independently selected from the group consisting of H, C<sub>1</sub>-C<sub>4</sub> alkyl, phenyl, perfluoroalkyl, and trimethylsilyl, subject to the proviso that in each NRR' group, R ≠ R';

5 (v) β-ketoimines of the formula



wherein each of R<sub>1</sub>, R<sub>2</sub>, R<sub>a</sub>, R<sub>b</sub>, R<sub>c</sub> and R<sub>d</sub> is independently selected from H, aryl, 10 C<sub>1</sub>-C<sub>6</sub> alkyl, and C<sub>1</sub>-C<sub>6</sub> perfluoroalkyl; and

(vi) tantalum cyclopentadienyl compounds of the formula:



wherein each R is independently selected from the group consisting of H, methyl, ethyl, isopropyl, t-butyl, and trimethylsilyl;

(vii)  $Ta(NR_1R_2)_x(NR_3R_4)_{5-x} / Ti(NR_1R_2)_x(NR_3R_4)_{4-x}$

5

where each of R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> and R<sub>4</sub> are independently selected from the group consisting of H, C<sub>1</sub>-C<sub>8</sub> alkyl, aryl, C<sub>1</sub>-C<sub>8</sub> perfluoroalkyl or a silicon-containing group selected from the group consisting of silane, alkylsilane, perfluoroalkylsilyl, triarylsilane and alkylsilylsilane;

10

(viii)  $Ta(NR_1)(NR_2R_3)_3$

15

where each of R<sub>1</sub>, R<sub>2</sub>, and R<sub>3</sub> are independently selected from the group consisting of H, C<sub>1</sub>-C<sub>8</sub> alkyl, aryl, C<sub>1</sub>-C<sub>8</sub> perfluoroalkyl or a silicon-containing group selected from the group consisting of silane, alkylsilane, perfluoroalkylsilyl, triarylsilane and alkylsilylsilane;

(ix)  $Ta(SiR_1R_2R_3)_x(NR_4R_5)_{5-x} / Ti(SiR_1R_2R_3)_x(NR_4R_5)_{4-x}$

20

where each of R<sub>1-5</sub> is independently selected from the group consisting of H, Me, Et, tBu, Ph, iPr, CF<sub>3</sub>, SiH<sub>3</sub>, SiMe<sub>3</sub>, Si(CF<sub>3</sub>)<sub>3</sub>, Si(Et)<sub>3</sub>, Si(iPr)<sub>3</sub>, Si(tBu)<sub>3</sub>, Si(Ph)<sub>3</sub>, and Si(SiMe<sub>3</sub>)<sub>x</sub>(Me)<sub>3-x</sub>; and

*Patent*  
 (x)  $(Cp^n)Ta(SiR_1R_2R_3)_x(NR_4R_5)_{4-x} / (Cp^n)_2Ti(SiR_1R_2R_3)(NR_4R_5)$

where each of  $R_{1-5}$  is independently selected from the group consisting of H, Me, Et,  $tBu$ ,  
 5 Ph,  $iPr$ ,  $CF_3$ ,  $SiH_3$ ,  $SiMe_3$ ,  $Si(CF_3)_3$ ,  $Si(Et)_3$ ,  $Si(iPr)_3$ ,  $Si(tBu)_3$ ,  $Si(Ph)_3$ ,  
 $Si(SiMe_3)_x(Me)_{3-x}$  and  $Cp^n$  is  $C_5H_xMe_{(5-x)}$  (where  $x = 0-5$ ).

2. A source reagent composition according to claim 1, further comprising a solvent for said tantalum and/or titanium species.

10

3. A source reagent composition according to claim 2, wherein said solvent is selected from the group consisting of  $C_6-C_{10}$  alkanes,  $C_6-C_{10}$  aromatics, and compatible mixtures thereof.

15

4. A source reagent composition according to claim 2, wherein said solvent is selected from the group consisting of hexane, heptane, octane, nonane, decane, toluene and xylene.

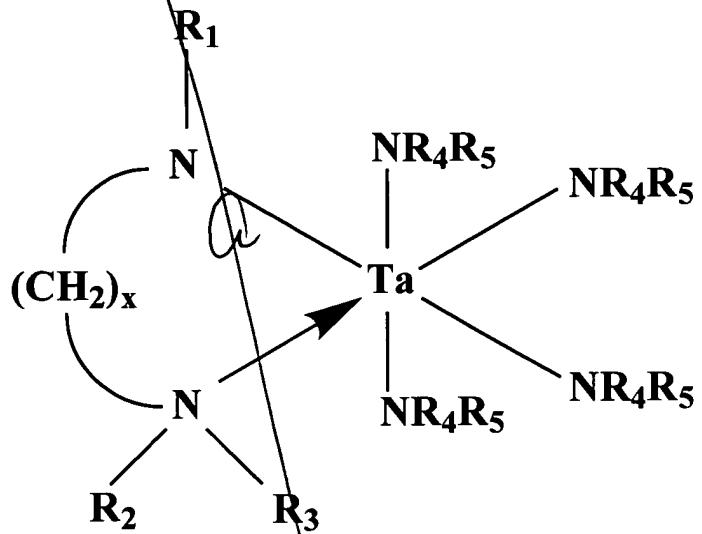
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5. A method of forming Ta or Ti material on a substrate from a precursor, comprising vaporizing said precursor to form a precursor vapor, and contacting the precursor vapor with the substrate to form said Ta or Ti material thereon, wherein the

precursor comprises at least one tantalum and/or titanium species selected from the group consisting of:

(i) tethered amine tantalum complexes of the formula:

5



wherein:

x is 2 or 3;

each of R<sub>1</sub>-R<sub>5</sub> is independently selected from the group consisting of H, C<sub>1</sub>-C<sub>4</sub>

10 alkyl, aryl, C<sub>1</sub>-C<sub>6</sub> perfluoroalkyl and trimethylsilyl;

(ii)  $\beta$ -diimines of the formula:



15

wherein:

G is a  $\beta$ -dilmino ligand;  
 each Q is selected from the group consisting of H, C<sub>1</sub>-C<sub>6</sub> alkyl, aryl and C<sub>1</sub>-C<sub>6</sub> perfluoroalkyl; and  
 x is an integer from 1 to 4 inclusive;

5

## (iii) tantalum diamide complexes of the formula



wherein:

10 x is 1 or 2;

y is 1 or 2;

each of R<sub>1</sub>-R<sub>4</sub> is independently selected from the group consisting of H, C<sub>1</sub>-C<sub>4</sub> alkyl, aryl, perfluoroalkyl, and trimethylsilyl;

## 15 (iv) tantalum amide compounds of the formula

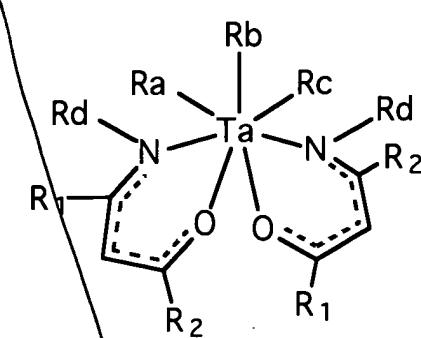


wherein each R and R' is independently selected from the group consisting of H, C<sub>1</sub>-C<sub>4</sub> alkyl, phenyl, perfluoroalkyl, and trimethylsilyl, subject to the proviso that in each

NRR' group, R  $\neq$  R';

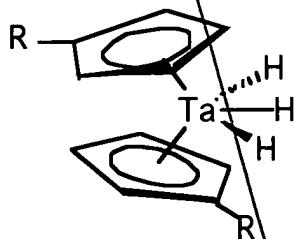
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(v)  $\beta$ -ketoimines of the formula



wherein each of  $R_1$ ,  $R_2$ ,  $R_a$ ,  $R_b$ ,  $R_c$  and  $R_d$  is independently selected from H, aryl, 5  $C_1$ - $C_6$  alkyl, and  $C_1$ - $C_6$  perfluoroalkyl; and

(vi) tantalum cyclopentadienyl compounds of the formula



wherein each R is independently selected from the group consisting of H, methyl, 10 ethyl, isopropyl, t-butyl, and trimethylsilyl;

(vii)  $Ta(NR_1R_2)_x(NR_3R_4)_{5-x}$  /  $Ti(NR_1R_2)_x(NR_3R_4)_{4-x}$

where each of  $R_1$ ,  $R_2$ ,  $R_3$  and  $R_4$  are independently selected from the group consisting of 15 H,  $C_1$ - $C_8$  alkyl, aryl,  $C_1$ - $C_8$  perfluoroalkyl or a silicon-containing group selected from the

group consisting of silane, alkylsilane, perfluoroalkylsilyl, triarylsilane and alkylsilylsilane;

(viii)  $Ta(NR_1)(NR_2R_3)_3$

5

where each of  $R_1$ ,  $R_2$ , and  $R_3$  are independently selected from the group consisting of H,  $C_1-C_8$  alkyl, aryl,  $C_1-C_8$  perfluoroalkyl or a silicon-containing group selected from the group consisting of silane, alkylsilane, perfluoroalkylsilyl, triarylsilane and alkylsilylsilane;

10

(ix)  $Ta(SiR_1R_2R_3)_x(NR_4R_5)_{5-x} / Ti(SiR_1R_2R_3)_x(NR_4R_5)_{4-x}$

where each of  $R_{1-5}$  is independently selected from the group consisting of H, Me, Et,  $t^3Bu$ , Ph,  $i^3Pr$ ,  $CF_3$ ,  $SiH_3$ ,  $SiMe_3$ ,  $Si(CF_3)_3$ ,  $Si(Et)_3$ ,  $Si(i^3Pr)_3$ ,  $Si(t^3Bu)_3$ ,  $Si(Ph)_3$ , and  $Si(SiMe_3)_x(Me)_{3-x}$ ; and

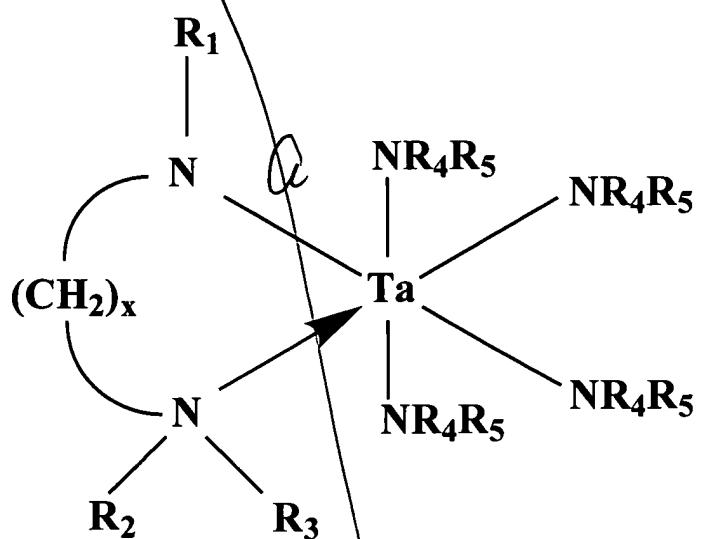
(x)  $(Cp^n)Ta(SiR_1R_2R_3)_x(NR_4R_5)_{4-x} / (Cp^n)_2Ti(SiR_1R_2R_3)(NR_4R_5)$

where each of  $R_{1-5}$  is independently selected from the group consisting of H, Me, Et,  $t^3Bu$ , Ph,  $i^3Pr$ ,  $CF_3$ ,  $SiH_3$ ,  $SiMe_3$ ,  $Si(CF_3)_3$ ,  $Si(Et)_3$ ,  $Si(i^3Pr)_3$ ,  $Si(t^3Bu)_3$ ,  $Si(Ph)_3$ ,  $Si(SiMe_3)_x(Me)_{3-x}$  and  $Cp^n$  is  $C_5H_xMe_{(5-x)}$  (where  $x = 0-5$ ).

6. A method according to claim 5, wherein said material formed on the substrate is TaN, and the precursor is selected from the group consisting of:

(i) tethered amine tantalum complexes of the formula:

5



wherein:

X is 2 or 3;

each of R<sub>1</sub>-R<sub>5</sub> is independently selected from the group consisting of H, C<sub>1</sub>-C<sub>4</sub>

10 alkyl, aryl, C<sub>1</sub>-C<sub>6</sub> perfluoroalkyl, and trimethylsilyl;

(ii)  $\beta$ -diimines of the formula:



15

wherein:

G is a  $\beta$ -diimino ligand;  
 each Q is selected from the group consisting of H, C<sub>1</sub>-C<sub>6</sub> alkyl, aryl and C<sub>1</sub>-C<sub>6</sub> perfluoroalkyl; and  
 x is an integer from 1 to 4 inclusive;

5

## (iii) tantalum diamide complexes of the formula



wherein:

10 x is 1 or 2;

y is 1 or 2;

each of R<sub>1</sub>-R<sub>4</sub> is independently selected from the group consisting of H, C<sub>1</sub>-C<sub>4</sub> alkyl, aryl, perfluoroalkyl, and trimethylsilyl;

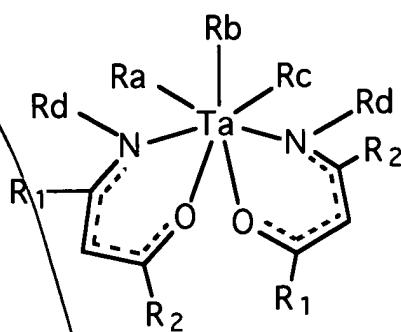
## 15 (iv) tantalum amide compounds of the formula



wherein each R and R' is independently selected from the group consisting of H, C<sub>1</sub>-C<sub>4</sub> alkyl, phenyl, perfluoroalkyl, and trimethylsilyl, subject to the proviso that in each NRR' group, R  $\neq$  R';

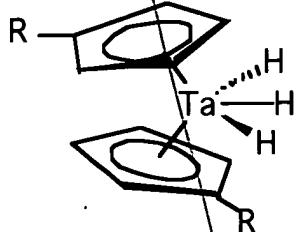
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(v)  $\beta$ -ketoimines of the formula



5 wherein each of  $R_1$ ,  $R_2$ ,  $R_a$ ,  $R_b$ ,  $R_c$  and  $R_d$  is independently selected from H, aryl,  $C_1$ - $C_6$  alkyl, and  $C_1$ - $C_6$  perfluoroalkyl; and

(vi) tantalum cyclopentadienyl compounds of the formula



10 wherein each R is independently selected from the group consisting of H, methyl, ethyl, isopropyl, t-butyl, trimethylsilyl.

7. A method according to claim 5, further comprising a solvent for said precursor.

8. A method according to claim 7, wherein said solvent is selected from the group consisting of C<sub>6</sub>-C<sub>10</sub> alkanes, C<sub>6</sub>-C<sub>10</sub> aromatics, and compatible mixtures thereof.

9. A method according to claim 7, wherein said solvent is selected from the 5 group consisting of hexane, heptane, octane, nonane, decane, toluene and xylene.

10. A method according to claim 5, comprising liquid delivery chemical vapor deposition of said precursor.

10 11. A method according to claim 5, comprising deposition of Ta and/or Ti on said substrate by a technique selected from the group consisting of chemical vapor deposition, assisted chemical vapor deposition, ion implantation, molecular beam epitaxy and rapid thermal processing.

15 12. A method according to claim 5, wherein the substrate comprises a microelectronic device structure.

13. A method according to claim 12, wherein TaN or TaSiN is deposited on said substrate, and the substrate thereafter is metallized with copper or integrated with a 20 ferroelectric thin film.

14. A method according to claim 12, wherein TaN is deposited on said substrate, and the substrate thereafter is metallized with copper or integrated with a ferroelectric thin film.

5 15. A method according to claim 5, comprising liquid delivery chemical vapor deposition of said precursor to form TaN on the substrate, and thereafter metallizing the substrate with copper or integrating the substrate with a ferroelectric thin film.